

Nov 18, 12 10:52	sup.txt	Page 1/18
Microsolvation of Mg <sup>2+</sup> , Ca <sup>2+</sup> : Strong influence of formal charges in hydrogen bonding networks		
Juan David Gonzalez Universidad de Antioquia, Colombia		
Elizabeth Florez Universidad de Medellin, Colombia		
Jonathan Romero, Andres Reyes Universidad Nacional de Colombia		
Albeiro Restrepo Universidad de Antioquia, Colombia		
Optimized Geometries at the MP2/6-311++G** level		
Cartesian coordinates for the [Ca(H <sub>2</sub> O) <sub>3</sub> ] <sup>2+</sup> clusters		
W3S1		
1	-2.461211000	-1.696379000 0.483640000
8	-1.621948000	-1.673376000 0.000368000
1	-1.619352000	-2.513212000 -0.482446000
1	-1.365120000	2.658975000 -0.485576000
8	-0.638678000	2.241064000 0.000302000
1	-0.241830000	2.978954000 0.486585000
1	2.986426000	-0.143394000 -0.480839000
8	2.260419000	-0.567488000 0.000304000
1	2.700185000	-1.283934000 0.481709000
20	0.000128000	-0.000130000 -0.000543000
W3S2		
1	0.195500000	-2.501678000 -0.000085000
8	0.150483000	-1.535545000 -0.000026000
1	1.083098000	-1.220850000 -0.000002000
1	3.012693000	-0.000022000 -0.760712000
8	2.413634000	-0.000001000 0.000027000
1	3.012709000	0.000024000 0.760753000
1	0.195489000	2.501679000 -0.000079000
8	0.150483000	1.535546000 -0.000029000
1	1.083103000	1.220865000 -0.000008000
20	-1.514970000	-0.000001000 0.000018000
W3S4		
1	-3.563387000	0.406765000 0.767637000
8	-2.995102000	0.216498000 0.005672000
1	-3.578632000	0.376201000 -0.751778000
1	3.952653000	-0.264529000 -0.758377000
8	3.362783000	-0.253124000 0.005470000
1	3.949281000	-0.256178000 0.771987000
1	2.019289000	0.466705000 -0.001458000
8	1.065897000	0.824508000 -0.005678000
1	1.165282000	1.786076000 -0.011005000
20	-0.770656000	-0.440905000 -0.003036000
W3S6		
1	-0.876129000	0.810587000 -0.000057000
8	-0.276822000	-0.000002000 -0.000052000
1	-0.876232000	-0.810519000 -0.000015000
1	-2.055411000	-2.564148000 -0.763491000
8	-1.583724000	-2.210280000 0.000010000
1	-2.055382000	-2.564138000 0.763533000
1	-2.055073000	2.564325000 0.763542000
8	-1.583422000	2.210465000 0.000015000
1	-2.055022000	2.564459000 -0.763481000
20	1.876250000	-0.000101000 0.000010000

Nov 18, 12 10:52	sup.txt	Page 2/18
Cartesian coordinates for the [Ca(H <sub>2</sub> O) <sub>4</sub> ] <sup>2+</sup> clusters		
W4S1		
1	1.337961000	2.673028000 0.578216000
8	1.422460000	1.722392000 0.735928000
1	2.235005000	1.650125000 1.255624000
1	-1.373767000	0.589735000 -2.651770000
8	-1.441052000	0.750000000 -1.700185000
1	-2.246584000	1.278692000 -1.615705000
1	2.208085000	-1.646142000 -1.308521000
8	1.409638000	-1.718184000 -0.767381000
1	1.332143000	-2.668261000 -0.602856000
1	-2.199422000	-1.285883000 1.669237000
8	-1.392850000	-0.755976000 1.733822000
1	-1.300612000	-0.598184000 2.683722000
20	0.001081000	0.001052000 -0.001271000
W4S2		
1	-2.959619000	-0.600245000 -0.495266000
8	-2.361875000	-0.006737000 -0.020217000
1	-2.960422000	0.584943000 0.455936000
1	-0.597989000	2.979113000 -0.390579000
8	0.003002000	2.361851000 0.048472000
1	0.612863000	2.940082000 0.526848000
1	2.963940000	0.581278000 -0.494745000
8	2.359127000	-0.006781000 -0.021905000
1	2.950524000	-0.602894000 0.457701000
1	-0.604243000	-2.936012000 0.526959000
8	0.002294000	-2.354830000 0.047938000
1	0.604901000	-2.969076000 -0.393200000
20	-0.001517000	0.003739000 -0.031397000
W4S3		
1	3.698433000	-0.000394000 0.762169000
8	3.100437000	-0.000163000 0.001408000
1	3.699582000	-0.000018000 -0.758449000
1	-3.812312000	-0.026042000 0.761788000
8	-3.212685000	-0.000119000 0.002041000
1	-3.814791000	0.025715000 -0.755747000
1	0.872770000	2.516180000 0.002632000
8	0.824154000	1.551447000 0.000702000
1	1.753499000	1.236173000 0.000671000
1	0.872553000	-2.516097000 -0.002970000
8	0.824008000	-1.551360000 -0.001297000
1	1.753380000	-1.236145000 0.000129000
20	-0.865521000	0.000109000 -0.001653000
W4S4		
1	2.250092000	-0.333787000 0.353616000
8	1.385161000	-0.511044000 0.840688000
1	1.651615000	-0.926087000 1.670753000
1	4.002393000	-0.656794000 -1.001677000
8	3.473002000	0.014699000 -0.555392000
1	4.096677000	0.720593000 -0.348107000
1	-1.132154000	2.954130000 0.499490000
8	-1.424286000	2.211950000 -0.049042000
1	-2.085385000	2.610593000 -0.632821000
1	-2.030560000	-2.656793000 -0.452304000
8	-2.215282000	-1.719068000 -0.298646000
1	-3.182266000	-1.677871000 -0.295790000
20	-0.665959000	-0.000314000 0.035299000

Nov 18, 12 10:52		sup.txt	Page 3/18
W4S5			
1	-2.891105000	0.301409000	-0.142971000
8	-2.000908000	0.758212000	-0.298104000
1	-2.229328000	1.652029000	-0.584668000
1	-4.722226000	-0.889108000	-0.548597000
8	-4.134296000	-0.570395000	0.146837000
1	-4.708746000	-0.424694000	0.908176000
1	4.721571000	-0.889641000	0.550985000
8	4.134595000	-0.570112000	-0.144881000
1	4.710091000	-0.423511000	-0.905258000
1	2.228574000	1.651312000	0.586889000
8	2.000561000	0.757859000	0.298870000
1	2.890977000	0.301303000	0.144267000
20	0.000028000	-0.214180000	-0.001530000
W4S6			
1	2.886851000	-0.492396000	-0.012732000
8	2.015969000	-1.008214000	-0.025925000
1	2.277707000	-1.937447000	-0.057403000
1	-4.643879000	-0.593631000	0.793083000
8	-4.067388000	-0.503660000	0.013090000
1	-4.647834000	-0.627154000	-0.759344000
1	4.643794000	0.595494000	0.792978000
8	4.067172000	0.505330000	0.013108000
1	4.647384000	0.629189000	-0.759442000
1	-2.886475000	0.493546000	-0.012624000
8	-2.015196000	1.008654000	-0.025708000
1	-2.276207000	1.938099000	-0.057006000
20	-0.000290000	-0.001129000	0.013798000
W4S7			
1	4.120020000	0.000974000	-0.758159000
8	3.517491000	0.000005000	0.000492000
1	4.119408000	-0.001178000	0.759629000
1	-1.616502000	0.802298000	0.000083000
8	-1.021312000	-0.000008000	0.000035000
1	-1.616506000	-0.802312000	0.000072000
1	-2.798152000	2.605056000	0.762508000
8	-2.329123000	2.246778000	0.000141000
1	-2.798787000	2.605104000	-0.761811000
1	-2.798937000	-2.604671000	0.762237000
8	-2.329147000	-2.246773000	0.000161000
1	-2.798055000	-2.605469000	-0.762083000
20	1.174212000	0.000009000	-0.000456000
W4S8			
1	0.301300000	-1.150917000	0.497145000
8	-0.577915000	-1.516532000	0.205189000
1	-0.503757000	-2.478884000	0.242329000
1	-0.505941000	2.479494000	0.240110000
8	-0.579268000	1.517042000	0.203895000
1	0.300235000	1.152467000	0.496266000
1	4.128897000	0.761902000	-0.848093000
8	3.561466000	-0.000712000	-0.691291000
1	4.129765000	-0.763603000	-0.843526000
1	1.811799000	0.002083000	1.782776000
8	1.475363000	0.001409000	0.876559000
1	2.296482000	0.001483000	0.304298000
20	-2.149797000	-0.000684000	-0.331306000

Nov 18, 12 10:52		sup.txt	Page 4/18
W4S10			
1	0.018430000	0.782034000	-0.342095000
8	-0.637828000	0.000212000	-0.298396000
1	0.018431000	-0.781626000	-0.342155000
1	1.350705000	-2.539228000	-0.761616000
8	1.153090000	-1.776682000	-0.208081000
1	2.008911000	-1.367414000	0.010277000
1	4.078304000	-0.000610000	-0.181946000
8	3.301462000	-0.000252000	0.391618000
1	3.680369000	0.000078000	1.279695000
1	2.009365000	1.367266000	0.009564000
8	1.153467000	1.776780000	-0.207999000
1	1.350847000	2.539827000	-0.760927000
20	-2.713844000	-0.000040000	0.183603000
Cartesian coordinates for the [Ca(H2O)5]2+ clusters			
W5S1			
1	2.890484000	0.011755000	-1.196158000
8	2.374575000	0.009422000	-0.379467000
1	3.045310000	0.012373000	0.315772000
1	0.774047000	-2.844691000	-0.878025000
8	0.010380000	-2.276552000	-0.715481000
1	-0.748251000	-2.851498000	-0.877660000
1	0.745956000	2.853051000	-0.879445000
8	-0.011809000	2.277251000	-0.716205000
1	-0.776303000	2.844539000	-0.877850000
1	0.003720000	-0.760166000	2.895562000
8	0.000068000	0.000642000	2.299975000
1	-0.003458000	0.761556000	2.895428000
1	-2.890027000	-0.013740000	-1.195661000
8	-2.373899000	-0.011594000	-0.379110000
1	-3.044424000	-0.015559000	0.316321000
20	0.000421000	0.000451000	-0.069799000
W5S2			
1	1.960863000	-0.271959000	-1.195692000
8	1.035068000	-0.332147000	-1.508489000
1	1.089792000	-0.488740000	-2.458966000
1	1.089466000	0.487557000	2.459090000
8	1.034855000	0.331506000	1.508518000
1	1.960690000	0.271510000	1.195792000
1	3.931114000	-0.741019000	0.169020000
8	3.333147000	-0.000060000	0.000150000
1	3.931007000	0.741000000	-0.168654000
1	-1.925371000	-2.784935000	-0.016676000
8	-2.096651000	-1.877738000	0.270249000
1	-2.951263000	-1.938571000	0.717988000
1	-1.924721000	2.784882000	0.020332000
8	-2.095082000	1.878686000	-0.270281000
1	-2.948236000	1.941076000	-0.720579000
20	-0.695202000	-0.000139000	-0.000141000
W5S3			
1	-4.312206000	0.708437000	0.760460000
8	-3.729727000	0.572787000	0.000183000
1	-4.312305000	0.707911000	-0.760111000
1	-0.982284000	2.519148000	-0.000855000
8	-1.152478000	1.568955000	-0.000470000
1	-2.127841000	1.472261000	-0.000277000
1	2.750470000	-1.818281000	-0.001743000
8	2.339773000	-0.944934000	-0.000860000
1	3.112549000	-0.302407000	-0.000308000
1	4.743456000	1.047010000	0.764750000
8	4.188593000	0.851152000	0.000804000
1	4.743469000	1.048510000	-0.762746000
1	-2.694212000	-0.942167000	0.000584000
8	-1.863386000	-1.462293000	0.000626000
1	-2.133089000	-2.389270000	0.000987000
20	0.147490000	-0.336824000	-0.000151000

Nov 18, 12 10:52		sup.txt	Page 5/18
W5S4			
1	3.169375000	2.066332000	-0.759035000
8	2.745436000	1.643810000	0.000174000
1	3.168715000	2.066485000	0.759666000
1	2.671780000	-0.150625000	0.000455000
8	2.294671000	-1.058258000	0.000578000
1	3.051045000	-1.657786000	0.001077000
1	-2.671788000	-0.150649000	0.000472000
8	-2.294668000	-1.058276000	0.000584000
1	-3.051036000	-1.657812000	0.001085000
1	-0.792522000	1.574517000	-0.000467000
8	-0.000018000	1.009429000	-0.000650000
1	0.792460000	1.574550000	-0.000463000
1	-3.169358000	2.066328000	-0.759050000
8	-2.745428000	1.643819000	0.000171000
1	-3.168711000	2.066509000	0.759651000
20	0.000005000	-1.262102000	-0.000512000
W5S5			
1	-0.697040000	3.508279000	0.301957000
8	0.000681000	2.910498000	-0.000285000
1	0.698704000	3.507801000	-0.302776000
1	4.433199000	-1.224137000	0.684200000
8	3.550204000	-1.571088000	0.511833000
1	3.646519000	-2.528176000	0.577916000
1	2.530202000	-0.875901000	-0.478341000
8	1.809624000	-0.396633000	-0.987110000
1	2.067982000	-0.474050000	-1.913483000
1	-2.530630000	-0.875078000	0.478418000
8	-1.810280000	-0.395361000	0.987090000
1	-2.069172000	-0.471788000	1.913396000
1	-4.433271000	-1.224292000	-0.684374000
8	-3.550287000	-1.571045000	-0.511550000
1	-3.646486000	-2.528185000	-0.577045000
20	0.000023000	0.568728000	0.000015000
W5S7			
1	3.202630000	-1.857443000	-0.759374000
8	2.642606000	-1.647359000	0.000051000
1	3.202592000	-1.857461000	0.759499000
1	1.781033000	0.167818000	0.000051000
8	0.971801000	0.705875000	0.000006000
1	1.256519000	1.663414000	-0.000009000
1	-0.239371000	-3.234079000	0.000018000
8	0.010730000	-2.302037000	-0.000030000
1	0.995504000	-2.284388000	-0.000020000
1	1.822682000	3.742537000	0.763422000
8	1.509126000	3.245035000	-0.000043000
1	1.823060000	3.742425000	-0.763425000
1	-4.093593000	-0.019379000	-0.000682000
8	-3.275582000	0.497436000	0.000058000
1	-3.589161000	1.412755000	0.000729000
20	-1.051567000	-0.273390000	-0.000028000
W5S9			
1	2.981938000	0.000201000	-0.163547000
8	2.226259000	0.000838000	-0.813927000
1	2.653320000	0.001446000	-1.680435000
1	1.003837000	1.170932000	-0.549484000
8	0.104641000	1.538397000	-0.350147000
1	0.190286000	2.498922000	-0.377581000
1	4.705605000	0.761114000	1.181592000
8	4.157546000	-0.000824000	0.965638000
1	4.705052000	-0.763429000	1.180638000
1	-4.424957000	0.757871000	0.611522000
8	-3.831833000	-0.000547000	0.513119000
1	-4.413272000	-0.759290000	0.664484000
1	1.003933000	-1.169853000	-0.551654000
8	0.104658000	-1.537725000	-0.353409000
1	0.189667000	-2.498161000	-0.385480000
20	-1.534279000	-0.000043000	0.018988000

Nov 18, 12 10:52		sup.txt	Page 6/18
W5S10			
1	1.992375000	0.419076000	1.791903000
8	1.708007000	0.239107000	0.886820000
1	2.450627000	0.583414000	0.321475000
1	3.804589000	2.037906000	-0.889439000
8	3.636677000	1.111923000	-0.685488000
1	4.491730000	0.681615000	-0.791449000
1	1.160088000	-2.840374000	0.355697000
8	0.621911000	-2.043912000	0.271417000
1	1.197351000	-1.272604000	0.552580000
1	-1.441861000	1.477969000	0.104987000
8	-0.929013000	0.618387000	0.117881000
1	-0.018381000	0.809090000	0.422594000
1	-2.425855000	3.383002000	-0.670392000
8	-2.439650000	2.713257000	0.022372000
1	-2.820191000	3.157389000	0.788375000
20	-1.458696000	-1.477329000	-0.344517000
W5S13			
1	-1.189283000	-1.293493000	0.323874000
8	-0.384725000	-1.750466000	0.000003000
1	-0.685683000	-2.462566000	-0.573217000
1	-3.196430000	0.001676000	0.369304000
8	-2.334483000	0.002063000	0.848864000
1	-2.587508000	0.003048000	1.779207000
1	0.713768000	0.784919000	-0.270528000
8	1.379054000	-0.000026000	-0.301782000
1	0.713012000	-0.784325000	-0.269898000
1	-0.683343000	2.464487000	-0.574800000
8	-0.383199000	1.752220000	-0.001364000
1	-1.188252000	1.296193000	0.322611000
1	-5.227773000	0.758338000	-0.629518000
8	-4.649320000	-0.002011000	-0.514772000
1	-5.228302000	-0.763086000	-0.621777000
20	3.477059000	-0.000971000	-0.005143000
Cartesian coordinates for the [Ca(H2O)6]2+ clusters			
W6S1			
1	-2.378790000	-0.950755000	1.719950000
8	-1.538227000	-0.480476000	1.775425000
1	-1.457597000	-0.247084000	2.708065000
1	-1.450444000	-2.037637000	-1.806366000
8	-1.450818000	-1.106010000	-1.555652000
1	-2.167887000	-0.720823000	-2.073560000
1	0.921553000	-2.735744000	1.088368000
8	1.130654000	-2.071718000	0.420438000
1	1.898469000	-2.431281000	-0.039949000
1	-0.920350000	2.736571000	-1.088405000
8	-1.130341000	2.072404000	-0.420890000
1	-1.898651000	2.432009000	0.038647000
1	1.458438000	0.244168000	-2.707566000
8	1.539270000	0.477483000	-1.774926000
1	2.380230000	0.947051000	-1.719448000
1	2.167279000	0.723567000	2.073357000
8	1.449797000	1.107917000	1.555399000
1	1.448549000	2.039616000	1.805843000
20	-0.000174000	0.000177000	0.000136000

Nov 18, 12 10:52	sup.txt	Page 7/18
W6S2		
1	-2.194768000	-1.232226000
8	-1.344542000	-1.290927000
1	-0.870552000	-1.983340000
1	2.112940000	1.335262000
8	1.168057000	1.583504000
1	1.150910000	2.546866000
1	1.480491000	-2.341690000
8	1.362869000	-1.413885000
1	2.265031000	-1.045697000
1	-1.297434000	-0.568074000
8	-1.619199000	-0.680933000
1	-2.432083000	-1.190854000
1	4.163459000	0.222897000
8	3.595776000	0.238071000
1	4.218124000	0.331421000
1	-2.393995000	2.162067000
8	-2.240217000	1.606970000
1	-2.913946000	1.894510000
20	-0.533506000	-0.023677000
W6S4		
1	-2.769120000	-0.694393000
8	-2.062888000	-0.148906000
1	-2.383729000	-0.020567000
1	2.182322000	0.892898000
8	1.881926000	0.464186000
1	2.627491000	-0.094748000
1	-1.366662000	3.112047000
8	-0.536840000	2.618550000
1	0.060852000	3.201047000
1	3.793528000	-2.128816000
8	3.544686000	-1.276227000
1	4.361744000	-0.962620000
1	1.999895000	-1.209696000
8	1.092034000	-0.939010000
1	0.898637000	-1.385772000
1	-4.635944000	-1.238960000
8	-3.791275000	-1.574950000
1	-3.949478000	-2.511198000
20	-0.092034000	0.494582000
W6S5		
1	-2.786509000	3.358292000
8	-2.351747000	2.884858000
1	-2.724588000	3.264059000
1	-1.766560000	1.361831000
8	-1.300419000	0.488185000
1	-1.987586000	-0.197279000
1	1.781548000	1.148019000
8	2.135039000	0.737560000
1	3.086161000	0.696317000
1	-3.053589000	-2.404825000
8	-2.546857000	-2.105353000
1	-3.066335000	-2.418058000
1	-0.783872000	-2.417689000
8	0.184383000	-2.256500000
1	0.597122000	-3.124548000
1	2.396437000	-0.185162000
8	2.292811000	0.365949000
1	2.850340000	1.133499000
20	0.907587000	-0.056602000

Nov 18, 12 10:52	sup.txt	Page 8/18
W6S6		
1	3.500566000	-2.477345000
8	2.648567000	-2.635118000
1	2.756252000	-3.474733000
1	-1.783443000	-0.155143000
8	-1.550401000	-0.698436000
1	-1.666589000	-1.604103000
1	-0.418533000	2.983784000
8	0.060893000	2.149229000
1	1.023024000	2.414976000
1	1.249757000	-2.136227000
8	0.380505000	-1.764049000
1	0.156516000	-2.295837000
1	3.100358000	3.019759000
8	2.605650000	2.708787000
1	3.047386000	3.111295000
1	-3.649182000	-0.118444000
8	-2.775738000	0.225818000
1	-2.919792000	0.687313000
20	-0.767606000	0.007743000
W6S8		
1	3.214751000	3.329590000
8	2.813176000	2.900372000
1	3.214961000	3.329507000
1	-2.545004000	2.094254000
8	-2.383896000	1.143244000
1	-3.296452000	0.730852000
1	2.451387000	-0.176638000
8	1.767157000	0.512592000
1	2.237302000	1.390790000
1	1.194394000	-2.420344000
8	0.227656000	-2.241628000
1	-0.203418000	-3.104374000
1	-5.237076000	-0.159328000
8	-4.650232000	-0.110613000
1	-5.236901000	-0.160409000
1	3.457962000	-2.432175000
8	2.949096000	-2.118423000
1	3.457673000	-2.432047000
20	-0.424662000	-0.033702000
W6S11		
1	3.685512000	-0.000282000
8	2.900668000	-0.000027000
1	3.284819000	-0.000173000
1	1.681191000	-1.175508000
8	0.793727000	-1.537461000
1	0.877940000	-2.497936000
1	5.481766000	0.761217000
8	4.924783000	-0.000774000
1	5.481731000	-0.762961000
1	-5.563463000	-0.764464000
8	-4.990409000	-0.000998000
1	-5.563763000	0.762064000
1	0.878512000	2.498442000
8	0.794081000	1.537988000
1	1.681446000	1.175794000
1	-3.779298000	-0.000067000
8	-2.928494000	0.000450000
1	-3.212227000	0.000821000
20	-0.844451000	0.000481000

Nov 18, 12 10:52		sup.txt	Page 9/18
W6S14			
1	-0.224409000	4.220008000	0.704863000
8	-0.465630000	3.657815000	-0.039192000
1	-0.526597000	4.257963000	-0.790277000
1	4.752263000	0.313112000	1.272813000
8	4.240367000	-0.443673000	0.969546000
1	4.825354000	-1.197799000	1.096350000
1	2.707123000	-0.242511000	-1.677930000
8	2.282939000	-0.338761000	-0.816396000
1	3.036929000	-0.368755000	-0.172613000
1	0.909688000	0.876983000	-0.423829000
8	-0.019564000	1.087800000	-0.204974000
1	-0.105033000	2.077152000	-0.155823000
1	-4.379261000	-0.154220000	0.726685000
8	-3.740064000	-0.852071000	0.526783000
1	-4.267243000	-1.661389000	0.578706000
1	0.446750000	-2.950211000	-0.609752000
8	0.278632000	-2.008615000	-0.490526000
1	1.142739000	-1.541288000	-0.656698000
20	-1.446587000	-0.622450000	0.027279000
Cartesian coordinates for the [Mg(H2O)3]2+ clusters			
W3S1			
1	-2.223140000	-1.448303000	-0.481754000
8	-1.380598000	-1.438901000	0.000067000
1	-1.355864000	-2.281225000	0.481727000
1	-1.303144000	2.311553000	0.477582000
8	-0.557282000	1.914239000	0.000149000
1	-0.141917000	2.650496000	-0.476825000
1	2.655137000	-0.026632000	0.475359000
8	1.937378000	-0.474971000	0.000045000
1	2.366435000	-1.204454000	-0.475227000
12	0.000543000	-0.000364000	-0.000245000
W3S3			
1	-1.792425000	0.220517000	0.000117000
8	-0.895203000	0.805332000	0.000212000
1	-1.176020000	1.732311000	0.001211000
1	-3.457333000	-0.710167000	-0.773138000
8	-2.885139000	-0.613717000	-0.000052000
1	-3.456676000	-0.711323000	0.773375000
1	3.363315000	-0.583502000	-0.771842000
8	2.799018000	-0.407243000	0.000219000
1	3.362550000	-0.583986000	0.772728000
12	0.917265000	0.196765000	-0.000457000
W3S5			
1	3.645766000	-0.701880000	-0.839496000
8	3.080205000	-0.600762000	-0.063095000
1	3.643114000	-0.712044000	0.713390000
1	0.269458000	0.517215000	0.113330000
8	-1.206945000	0.000698000	0.518496000
1	-1.120484000	-0.213646000	1.456571000
1	1.313856000	1.768304000	0.143442000
8	1.161680000	0.871970000	-0.186057000
1	2.033012000	0.228918000	-0.093891000
12	-2.838686000	-0.255176000	-0.304009000
W3S6			
1	-0.843048000	-0.440047000	0.000001000
8	0.000001000	0.158013000	0.000000000
1	0.843051000	-0.440046000	-0.000006000
1	2.478504000	-1.613398000	-0.768241000
8	2.133847000	-1.140621000	-0.000006000
1	2.478175000	-1.613356000	0.768404000
1	-2.478530000	-1.613347000	0.768260000
8	-2.133846000	-1.140624000	0.000004000
1	-2.478147000	-1.613412000	-0.768385000
12	-0.000002000	2.026622000	-0.000002000

Nov 18, 12 10:52		sup.txt	Page 10/18
Cartesian coordinates for the [Mg(H2O)4]2+ clusters			
W4S1			
1	2.015522000	1.824413000	-0.198824000
8	1.206441000	1.500287000	-0.620234000
1	1.105343000	2.036198000	-1.420340000
1	-2.024558000	-0.201855000	-1.813300000
8	-1.211662000	-0.620912000	-1.495737000
1	-1.111205000	-1.419358000	-2.034237000
1	-2.016194000	0.191956000	1.824099000
8	-1.209301000	0.616854000	1.499086000
1	-1.112870000	1.419065000	2.032695000
1	2.025172000	-1.814545000	0.194727000
8	1.214265000	-1.496005000	0.616881000
1	1.117131000	-2.033224000	1.416593000
12	0.000309000	-0.000370000	-0.000115000
W4S3			
1	-1.419907000	-1.229379000	0.000066000
8	-0.465609000	-1.474247000	-0.000138000
1	-0.401392000	-2.439218000	-0.000385000
1	-1.419751000	1.230347000	-0.000045000
8	-0.465420000	1.474808000	-0.000087000
1	-0.400901000	2.439765000	-0.000016000
1	-3.346857000	-0.000443000	-0.761003000
8	-2.747588000	-0.000338000	0.000145000
1	-3.346807000	-0.000503000	0.761333000
1	3.431933000	-0.001347000	0.770674000
8	2.842336000	-0.000373000	0.000120000
1	3.432072000	0.000355000	-0.770328000
12	0.846821000	0.000135000	-0.000052000
W4S4			
1	3.699513000	-0.138900000	0.993013000
8	3.188873000	0.042068000	0.193879000
1	3.843430000	0.202139000	-0.497524000
1	-2.708775000	-1.721814000	0.732609000
8	-2.510121000	-0.962637000	0.162861000
1	-3.338531000	-0.772808000	-0.303792000
1	1.076619000	-1.885643000	-0.565045000
8	0.950453000	-0.976568000	-0.261750000
1	1.894290000	-0.600757000	-0.079780000
1	-1.532775000	2.500392000	0.381949000
8	-0.855280000	1.949080000	-0.038318000
1	-0.222541000	2.573164000	-0.425391000
12	-0.741885000	-0.047609000	-0.057451000
W4S6			
1	-2.630740000	0.015084000	-0.262952000
8	-1.811217000	-0.523495000	-0.643469000
1	-2.148725000	-1.049365000	-1.382364000
1	-4.366497000	0.387838000	0.857661000
8	-3.661422000	0.784333000	0.329839000
1	-4.055492000	1.549480000	-0.108469000
1	2.630593000	0.016134000	0.263400000
8	1.810629000	-0.520750000	0.645348000
1	2.147292000	-1.043459000	1.386866000
1	4.055586000	1.549761000	0.103765000
8	3.661959000	0.782736000	-0.331651000
1	4.367592000	0.383928000	-0.856979000
12	0.000066000	-0.499332000	-0.000122000

Nov 18, 12 10:52		sup.txt		Page 11/18
W4S7				
1	3.816783000	0.002688000	-0.771202000	
8	3.226306000	-0.000060000	0.000363000	
1	3.816037000	-0.002838000	0.772498000	
1	-1.232903000	0.829108000	0.000008000	
8	-0.641408000	0.000009000	-0.000142000	
1	-1.232922000	-0.829058000	-0.000045000	
1	-2.413065000	2.522350000	0.766706000	
8	-1.946221000	2.167994000	0.000244000	
1	-2.413455000	2.522193000	-0.766053000	
1	-2.413345000	-2.522228000	0.766492000	
8	-1.946413000	-2.167910000	0.000068000	
1	-2.413531000	-2.522183000	-0.766264000	
12	1.245691000	-0.000025000	-0.000533000	
W4S9				
1	4.350540000	1.375563000	-0.422731000	
8	3.887593000	0.765227000	0.163727000	
1	4.525523000	0.496568000	0.835321000	
1	0.045508000	-0.974082000	1.446478000	
8	-0.149849000	-0.598766000	0.579188000	
1	1.135332000	-0.600778000	-0.132075000	
1	-4.145621000	1.370211000	-0.137235000	
8	-3.740039000	0.499988000	-0.280166000	
1	-4.438651000	-0.045786000	-0.675649000	
1	2.824814000	-0.043511000	-0.304475000	
8	2.013341000	-0.588551000	-0.686733000	
1	2.281524000	-1.472483000	-0.971356000	
12	-1.888944000	-0.060741000	0.179466000	
W4S10				
1	-0.412519000	0.815656000	-0.269831000	
8	-1.080006000	0.000031000	-0.218930000	
1	-0.412498000	-0.815598000	-0.269839000	
1	0.785903000	-2.488591000	-0.798329000	
8	0.638621000	-1.755410000	-0.189975000	
1	1.509944000	-1.357447000	-0.003083000	
1	3.554172000	-0.000153000	-0.252337000	
8	2.787774000	-0.000044000	0.336381000	
1	3.184505000	0.000069000	1.217546000	
1	1.510046000	1.357396000	-0.003320000	
8	0.638701000	1.755420000	-0.189970000	
1	0.785899000	2.488775000	-0.798135000	
12	-2.865514000	-0.000007000	0.273107000	
Cartesian coordinates for the [Mg(H2O)5]2+ clusters				
W5S1				
1	0.769699000	-2.494425000	-0.908448000	
8	-0.000299000	-1.940236000	-0.727515000	
1	-0.770399000	-2.494803000	-0.906837000	
1	-2.707279000	0.001054000	0.504665000	
8	-2.093952000	0.000378000	-0.241984000	
1	-2.654433000	-0.000158000	-1.029221000	
1	-0.000092000	-0.771329000	2.572711000	
8	0.000605000	-0.001690000	1.987844000	
1	0.001688000	0.766846000	2.574158000	
1	2.707344000	-0.001769000	0.503762000	
8	2.093863000	0.000299000	-0.242756000	
1	2.654182000	0.002248000	-1.030108000	
1	0.769629000	2.496167000	-0.904309000	
8	-0.000246000	1.941158000	-0.725386000	
1	-0.770466000	2.495583000	-0.904638000	
12	0.000031000	0.000109000	-0.072780000	

Nov 18, 12 10:52		sup.txt		Page 12/18
W5S2				
1	3.629960000	0.636060000	-0.417046000	
8	3.031534000	-0.000027000	0.000033000	
1	3.629784000	-0.636228000	0.417193000	
1	-2.758490000	-1.336542000	1.130829000	
8	-1.917470000	-1.442276000	0.664717000	
1	-1.756100000	-2.396044000	0.642735000	
1	-1.755307000	2.396244000	-0.642839000	
8	-1.916996000	1.442531000	-0.664824000	
1	-2.758042000	1.337077000	-1.130952000	
1	1.665066000	-0.661944000	-1.003025000	
8	0.716476000	-0.798760000	-1.216514000	
1	0.670218000	-1.226139000	-2.080900000	
1	1.665043000	0.661852000	1.003101000	
8	0.716442000	0.798588000	1.216587000	
1	0.670144000	1.225973000	2.080968000	
12	-0.661847000	-0.000062000	-0.000005000	
W5S3				
1	-2.302765000	1.814564000	-0.002549000	
8	-1.945814000	0.916802000	-0.001228000	
1	-2.756200000	0.285066000	-0.000409000	
1	-4.407389000	-0.882386000	-0.766061000	
8	-3.844135000	-0.724079000	0.001462000	
1	-4.406648000	-0.880859000	0.769841000	
1	0.460005000	-2.295344000	-0.001957000	
8	0.792635000	-1.388248000	-0.001189000	
1	1.775514000	-1.423077000	-0.000608000	
1	2.464667000	0.927177000	0.001102000	
8	1.619625000	1.430817000	0.000874000	
1	1.833172000	2.373277000	0.001606000	
1	3.983033000	-0.788386000	-0.760287000	
8	3.407867000	-0.622276000	0.000738000	
1	3.982284000	-0.789298000	0.762130000	
12	-0.072257000	0.396261000	-0.000673000	
W5S5				
1	-0.753833000	3.331050000	0.161604000	
8	-0.000176000	2.745166000	-0.000002000	
1	0.753361000	3.331200000	-0.161618000	
1	3.937707000	-1.476337000	0.780506000	
8	3.067791000	-1.696539000	0.426043000	
1	3.103805000	-2.639333000	0.225011000	
1	2.227149000	-0.728342000	-0.336860000	
8	1.602676000	-0.051550000	-0.786677000	
1	1.952886000	0.092581000	-1.674988000	
1	-2.227045000	-0.728526000	0.336872000	
8	-1.602554000	-0.051804000	0.786765000	
1	-1.952721000	0.092194000	1.675114000	
1	-3.937616000	-1.476532000	-0.780754000	
8	-3.067723000	-1.696604000	-0.426156000	
1	-3.103677000	-2.639372000	-0.224989000	
12	-0.000010000	0.737672000	0.000026000	
W5S6				
1	4.386975000	0.768235000	-1.030560000	
8	3.833941000	-0.000156000	-0.843835000	
1	4.387371000	-0.768139000	-1.031070000	
1	2.352346000	0.000653000	1.732360000	
8	1.979495000	0.000226000	0.840994000	
1	2.777084000	-0.000472000	0.191413000	
1	-1.147233000	-2.426423000	0.077164000	
8	-1.208660000	-1.462380000	0.054098000	
1	-2.137555000	-1.219720000	-0.159004000	
1	-1.146206000	2.426375000	0.077199000	
8	-1.208069000	1.462363000	0.053976000	
1	-2.137011000	1.220185000	-0.159369000	
1	-4.200445000	0.000449000	0.152734000	
8	-3.448804000	0.000211000	-0.457630000	
1	-3.864397000	0.000100000	-1.332110000	
12	0.095488000	-0.000280000	0.358368000	

Nov 18, 12 10:52		sup.txt	Page 13/18
W5S7			
1	2.472743000	-2.492890000	-0.759093000
8	2.139437000	-1.996255000	0.001220000
1	2.473076000	-2.491517000	0.762283000
1	-3.496989000	-1.858533000	-0.765877000
8	-3.033714000	-1.499143000	0.000026000
1	-3.498088000	-1.853624000	0.767550000
1	0.001214000	-1.582242000	0.000538000
8	-0.596605000	-0.817986000	0.000173000
1	-1.555530000	-1.155307000	0.000212000
1	-0.387453000	3.622133000	0.027747000
8	-0.782299000	2.737491000	0.000966000
1	-1.739594000	2.886370000	-0.024707000
1	2.349910000	-0.332864000	-0.000693000
8	2.094509000	0.629013000	-0.001780000
1	2.900012000	1.161276000	-0.004830000
12	0.159173000	0.972686000	-0.000664000
W5S8			
1	-4.806149000	-1.100328000	-0.137707000
8	-4.158434000	-0.606632000	-0.652007000
1	-4.605201000	-0.387204000	-1.476798000
1	2.219084000	2.510874000	-0.156316000
8	2.352162000	1.624344000	-0.523573000
1	2.944201000	1.746697000	-1.279861000
1	-3.012396000	0.281210000	-0.057001000
8	-2.253059000	0.846930000	0.280923000
1	-2.623625000	1.556766000	0.818105000
1	2.425789000	-2.542580000	-0.377104000
8	2.702029000	-1.622514000	-0.251160000
1	3.669631000	-1.639452000	-0.284572000
1	-1.224566000	0.316399000	0.684873000
8	-0.206014000	-0.154125000	1.001205000
1	-0.371859000	-0.649914000	1.811773000
12	1.490968000	-0.066374000	0.134292000
W5S11			
1	-2.992284000	1.825321000	-0.396798000
8	-2.790403000	0.881524000	-0.439736000
1	-3.649454000	0.313377000	-0.326904000
1	2.941178000	-1.764023000	-0.566100000
8	2.693553000	-0.880443000	-0.262483000
1	3.557911000	-0.311628000	-0.272758000
1	-5.280601000	-0.856006000	-1.021228000
8	-4.821016000	-0.538587000	-0.235176000
1	-5.483507000	-0.496924000	0.463870000
1	-0.998851000	0.308985000	1.765145000
8	-0.776907000	0.251322000	0.828225000
1	-1.941075000	0.611598000	0.138564000
1	5.120065000	0.944638000	-1.034837000
8	4.704596000	0.591331000	-0.238683000
1	5.410473000	0.519908000	0.415585000
12	0.936463000	-0.294702000	0.301523000
W5S13			
1	-0.682052000	-1.273126000	0.323621000
8	0.132973000	-1.722579000	0.003214000
1	-0.139888000	-2.403270000	-0.621950000
1	-2.673479000	0.000326000	0.362785000
8	-1.804341000	0.000613000	0.836863000
1	-2.048523000	0.001103000	1.770420000
1	1.150474000	0.821728000	-0.231572000
8	1.833148000	-0.000164000	-0.284057000
1	1.149968000	-0.821794000	-0.231311000
1	-0.138837000	2.404144000	-0.622236000
8	0.133611000	1.723154000	0.002780000
1	-0.681673000	1.274132000	0.323064000
1	-4.682875000	0.760706000	-0.615709000
8	-4.103383000	-0.000558000	-0.509924000
1	-4.683321000	-0.761817000	-0.613287000
12	3.657845000	-0.000488000	-0.019569000

Nov 18, 12 10:52		sup.txt	Page 14/18
Cartesian coordinates for the [Mg(H2O)6]2+ clusters			
W6S1			
1	-0.989332000	2.433335000	-0.952120000
8	-0.979072000	1.483970000	-1.123962000
1	-1.511537000	1.356447000	-1.918413000
1	1.539185000	1.965647000	1.253810000
8	0.712990000	1.472038000	1.322271000
1	0.281780000	1.794070000	2.123072000
1	1.837712000	0.841951000	-1.928857000
8	1.719280000	0.234551000	-1.188611000
1	2.553394000	-0.243445000	-1.106738000
1	-1.837839000	-0.842422000	1.928582000
8	-1.719562000	-0.234764000	1.188518000
1	-2.553627000	0.243415000	1.107187000
1	1.511796000	-1.355711000	1.918403000
8	0.980012000	-1.483523000	1.123544000
1	0.990374000	-2.432953000	0.952064000
1	-0.282440000	-1.794302000	-2.122787000
8	-0.713396000	-1.472263000	-1.321850000
1	-1.539761000	-1.965573000	-1.253323000
12	-0.000143000	-0.000045000	-0.000013000
W6S2			
1	0.803780000	-1.607602000	-2.208766000
8	1.301131000	-1.006916000	-1.639566000
1	2.200041000	-1.001328000	-1.990868000
1	-1.831164000	1.268187000	-0.035142000
8	-0.868173000	1.442745000	-0.025295000
1	-0.748937000	2.398854000	-0.033516000
1	-1.995037000	-1.003994000	0.056463000
8	-1.069622000	-1.320660000	0.088719000
1	-1.101363000	-2.270874000	0.247000000
1	2.387284000	1.858716000	-0.937434000
8	2.086854000	1.383012000	-0.152595000
1	2.568181000	1.780400000	0.584265000
1	0.889272000	-0.966702000	2.552621000
8	1.376401000	-0.713126000	1.758254000
1	2.295003000	-0.952612000	1.934364000
1	-3.950085000	0.322331000	0.706558000
8	-3.335112000	0.241966000	-0.035131000
1	-3.908874000	0.256015000	-0.813168000
12	0.538339000	-0.024797000	-0.001456000
W6S3			
1	4.325765000	-0.539571000	-0.536662000
8	3.728489000	-0.000128000	-0.000031000
1	4.325859000	0.539243000	0.536568000
1	-4.325797000	-0.536749000	0.539348000
8	-3.728489000	-0.000121000	-0.000062000
1	-4.325827000	0.536444000	-0.539502000
1	1.339349000	-1.695847000	1.705649000
8	1.396528000	-1.017063000	1.022489000
1	2.346010000	-0.845509000	0.849839000
1	1.339631000	1.696126000	-1.705340000
8	1.396689000	1.017153000	-1.022357000
1	2.346145000	0.845383000	-0.849740000
1	-1.339678000	1.705610000	1.695866000
8	-1.396716000	1.022495000	1.017024000
1	-2.346166000	0.849733000	0.845376000
1	-1.339299000	-1.705537000	-1.695949000
8	-1.396501000	-1.022451000	-1.017093000
1	-2.345989000	-0.849911000	-0.845458000
12	0.000000000	0.000125000	0.000021000

Nov 18, 12 10:52		sup.txt	Page 15/18
W6S4			
1	-2.015498000	0.335864000	1.840426000
8	-1.742954000	0.114493000	0.942340000
1	-2.457593000	-0.496693000	0.571865000
1	1.948484000	1.177088000	1.892109000
8	1.666486000	0.631493000	1.148295000
1	2.391550000	0.002606000	0.947712000
1	-4.338218000	-1.099505000	-0.433003000
8	-3.482642000	-1.432685000	-0.109784000
1	-3.649066000	-2.336472000	0.210719000
1	1.633994000	-1.204728000	-0.984772000
8	0.748767000	-0.830789000	-1.177807000
1	0.414049000	-1.258893000	-1.974627000
1	3.369247000	-2.169214000	0.434912000
8	3.183572000	-1.325156000	-0.018746000
1	4.011091000	-1.099537000	-0.484807000
1	0.231563000	2.866336000	-1.372789000
8	-0.377987000	2.326793000	-0.852125000
1	-1.213491000	2.812071000	-0.841766000
12	-0.024004000	0.549824000	0.061387000
W6S5			
1	3.397022000	-2.365666000	0.475467000
8	2.814285000	-2.041403000	-0.220257000
1	3.252213000	-2.282311000	-1.044179000
1	1.829170000	-0.822763000	-0.055061000
8	1.133982000	-0.108821000	0.054797000
1	1.579467000	0.754271000	0.063367000
1	-0.976854000	-1.574263000	2.346430000
8	-1.504813000	-1.299962000	1.584458000
1	-2.404860000	-1.597286000	1.773335000
1	1.726296000	3.238871000	0.823724000
8	1.380899000	2.760469000	0.057907000
1	1.747493000	3.241821000	-0.696096000
1	-0.319426000	2.366971000	0.028834000
8	-1.125223000	1.798641000	0.014319000
1	-1.893022000	2.370379000	0.130113000
1	-2.229536000	-0.467326000	-2.281750000
8	-1.898575000	-0.957760000	-1.517092000
1	-2.100878000	-1.885343000	-1.698616000
12	-0.834294000	-0.182223000	0.028448000
W6S6			
1	3.288285000	-2.096476000	-0.375105000
8	2.430324000	-2.343966000	-0.012351000
1	2.549966000	-3.240148000	0.322251000
1	-1.554336000	-0.180187000	2.611671000
8	-1.391282000	-0.696557000	1.811162000
1	-1.420554000	-1.621797000	2.088232000
1	-0.612850000	2.653467000	0.203121000
8	-0.116186000	1.832324000	0.110340000
1	0.856742000	2.097385000	0.075380000
1	1.082253000	-1.807565000	-0.567802000
8	0.199011000	-1.430499000	-0.874976000
1	-0.003810000	-1.867948000	-1.710037000
1	2.878220000	2.715933000	0.779652000
8	2.373835000	2.423217000	0.011876000
1	2.779504000	2.871403000	-0.739229000
1	-3.488327000	-0.182499000	-0.766654000
8	-2.638217000	0.202044000	-1.018973000
1	-2.812649000	0.706124000	-1.825005000
12	-0.866861000	0.004984000	-0.026091000

Nov 18, 12 10:52		sup.txt	Page 16/18
W6S7			
1	-4.762242000	1.050290000	0.414868000
8	-4.196209000	0.643046000	-0.249514000
1	-4.756181000	0.557378000	-1.028458000
1	3.804220000	-0.920025000	0.557747000
8	2.959358000	-1.113400000	0.129163000
1	3.019658000	-2.036784000	-0.152292000
1	-0.014701000	-0.965321000	-2.203308000
8	0.000990000	-0.770222000	-1.259362000
1	-0.909289000	-0.920969000	-0.893381000
1	-0.927518000	-0.183836000	1.255668000
8	-0.023982000	0.170295000	1.463246000
1	0.014771000	0.370174000	2.405566000
1	-2.501155000	-1.739760000	0.568862000
8	-2.138826000	-0.890358000	0.284927000
1	-2.940719000	-0.329455000	0.089002000
1	2.867831000	2.132795000	-0.896823000
8	2.100743000	1.897755000	-0.357253000
1	1.719850000	2.739398000	-0.071036000
12	1.314073000	0.062433000	-0.011339000
W6S8			
1	-3.088526000	3.148801000	-0.765388000
8	-2.670859000	2.739154000	0.000856000
1	-3.088636000	3.148337000	0.767285000
1	1.983969000	2.051678000	-0.002376000
8	1.932045000	1.087632000	-0.001228000
1	2.892961000	0.745101000	-0.000640000
1	-2.239024000	-0.281528000	-0.001982000
8	-1.585012000	0.435925000	-0.000772000
1	-2.072465000	1.321232000	-0.000096000
1	-0.706051000	-2.364529000	0.000877000
8	0.205511000	-1.978307000	0.001068000
1	0.845694000	-2.700090000	0.001838000
1	4.843992000	0.126260000	0.767543000
8	4.259337000	0.107638000	0.000396000
1	4.844279000	0.124246000	-0.766579000
1	-2.874024000	-2.751944000	0.759922000
8	-2.421767000	-2.361786000	-0.000613000
1	-2.872689000	-2.753875000	-0.760949000
12	0.314707000	-0.004645000	0.000240000
W6S9			
1	4.279188000	-0.194491000	0.803159000
8	3.692288000	-0.214305000	0.023667000
1	4.294546000	-0.181379000	-0.743748000
1	-2.608326000	-0.537599000	-0.000580000
8	-1.730561000	-0.028338000	-0.014269000
1	-1.916479000	0.926184000	-0.012851000
1	-1.226545000	3.325701000	-0.772851000
8	-1.015893000	2.765961000	-0.002315000
1	-1.236108000	3.318968000	0.770780000
1	1.697156000	-2.793048000	-0.025462000
8	1.613446000	-1.831543000	-0.016005000
1	2.521632000	-1.427623000	-0.001197000
1	0.641190000	2.017115000	0.004592000
8	1.131501000	1.168553000	0.001502000
1	2.089374000	1.305943000	0.012858000
1	-4.422019000	-1.523833000	0.809474000
8	-3.863359000	-1.400710000	0.022376000
1	-4.436934000	-1.541358000	-0.750783000
12	0.141995000	-0.530961000	-0.017754000



Nov 18, 12 10:52		sup.txt	Page 17/18
W6S10			
1	3.853828000	-1.734954000	0.156245000
8	3.212379000	-1.366349000	-0.480224000
1	3.461368000	-1.744797000	-1.344369000
1	0.149519000	2.469728000	-0.499618000
8	0.456142000	1.612904000	-0.180216000
1	1.473032000	1.653646000	-0.113268000
1	0.476432000	-2.436627000	0.453830000
8	0.679801000	-1.515903000	0.246180000
1	1.640083000	-1.493949000	-0.031825000
1	-3.235544000	-0.099968000	0.201183000
8	-2.435465000	-0.135350000	0.837162000
1	-2.799059000	-0.219981000	1.727545000
1	3.583582000	2.234847000	0.156068000
8	2.958004000	1.492970000	0.088404000
1	3.416559000	0.739627000	-0.329292000
1	-4.935787000	0.719297000	-0.899433000
8	-4.327426000	-0.037533000	-0.827532000
1	-4.837666000	-0.826039000	-1.084240000
12	-0.549486000	0.027772000	0.344748000
W6S11			
1	3.359654000	-0.000192000	-0.364813000
8	2.527642000	-0.000320000	-0.919647000
1	2.843170000	-0.000692000	-1.833160000
1	1.348425000	-1.144906000	-0.505762000
8	0.454853000	-1.442418000	-0.184976000
1	0.429629000	-2.406784000	-0.174723000
1	5.215529000	0.762834000	0.757826000
8	4.647843000	-0.000134000	0.605014000
1	5.215247000	-0.763208000	0.758351000
1	-5.221545000	-0.768766000	-0.675308000
8	-4.653557000	-0.000800000	-0.540415000
1	-5.221635000	0.766836000	-0.676796000
1	0.429287000	2.407098000	-0.176190000
8	0.454704000	1.442728000	-0.185878000
1	1.348301000	1.145266000	-0.506452000
1	-3.490636000	0.000178000	0.395426000
8	-2.634284000	0.000762000	0.957339000
1	-2.911782000	0.001558000	1.882366000
12	-0.810105000	0.000186000	0.272312000
W6S12			
1	5.224436000	0.767207000	-0.670586000
8	4.656070000	-0.000874000	-0.537726000
1	5.224062000	0.768501000	-0.674737000
1	3.491255000	-0.002479000	0.394477000
8	2.634316000	-0.002263000	0.955980000
1	2.911469000	-0.004104000	1.881142000
1	-5.215286000	0.757696000	0.765756000
8	-4.647747000	-0.004067000	0.606245000
1	-5.214992000	-0.768346000	0.754332000
1	-1.349717000	-1.141313000	-0.508289000
8	-0.456060000	-1.440577000	-0.188898000
1	-0.431653000	-2.405021000	-0.181596000
1	-3.360435000	0.002874000	-0.363166000
8	-2.528649000	0.003669000	-0.918690000
1	-2.844825000	0.005756000	-1.832025000
1	-0.429914000	2.408157000	-0.173422000
8	-0.455071000	1.443763000	-0.183862000
1	-1.348876000	1.146081000	-0.504351000
12	0.810133000	0.000398000	0.270673000

Nov 18, 12 10:52		sup.txt	Page 18/18
W6S13			
1	-2.338295000	1.277248000	0.344660000
8	-1.520259000	1.758586000	0.567462000
1	-1.789571000	2.573780000	1.005155000
1	0.798735000	2.151999000	-1.334869000
8	0.653413000	1.505610000	-0.634356000
1	-0.267645000	1.685429000	-0.216459000
1	-1.788115000	-2.574706000	-1.004450000
8	-1.519339000	-1.759080000	-0.567234000
1	-2.337669000	-1.277740000	-0.345510000
1	0.798287000	-2.149805000	1.337485000
8	0.653411000	-1.504453000	0.635924000
1	-0.267309000	-1.684946000	0.217609000
1	-4.245065000	-0.181727000	0.736118000
8	-3.647242000	-0.000443000	-0.000962000
1	-4.244660000	0.180644000	-0.738419000
1	4.297280000	0.769294000	0.011655000
8	3.709892000	-0.000593000	-0.001105000
1	4.296356000	-0.771172000	-0.014650000
12	1.704055000	0.000390000	0.000321000
W6S14			
1	1.530481000	3.804937000	-0.728341000
8	1.635058000	3.193274000	0.009370000
1	1.878527000	3.744239000	0.762093000
1	-4.406207000	1.065738000	-1.115765000
8	-4.018354000	0.220555000	-0.865679000
1	-4.718847000	-0.423117000	-1.015914000
1	-2.421077000	0.029228000	1.720913000
8	-2.043001000	-0.085220000	0.839473000
1	-2.812497000	0.040857000	0.218885000
1	-0.447325000	0.963929000	0.433652000
8	0.497263000	0.917339000	0.190102000
1	0.883452000	1.847114000	0.132488000
1	3.831304000	-0.874427000	-0.720076000
8	3.075223000	-1.446857000	-0.522155000
1	3.409364000	-2.351987000	-0.609380000
1	-0.590588000	-2.879332000	0.437542000
8	-0.353252000	-1.946745000	0.379655000
1	-1.159472000	-1.378869000	0.601243000
12	1.223283000	-0.867257000	-0.030289000
W6S15			
1	-2.477872000	0.846205000	0.375472000
8	-1.975005000	-0.021593000	0.301479000
1	-2.562585000	-0.770019000	-0.023550000
1	2.371394000	-2.465316000	0.924056000
8	2.710050000	-1.559054000	0.949056000
1	3.392794000	-1.556949000	1.633877000
1	0.092902000	0.343746000	-1.742780000
8	0.257183000	0.137883000	-0.816860000
1	-1.067216000	0.052681000	-0.192349000
1	-3.878611000	-2.559961000	0.186980000
8	-3.430005000	-1.995632000	-0.451771000
1	-3.935771000	-2.080195000	-1.266776000
1	-3.733570000	2.679649000	-0.071539000
8	-3.206379000	2.210389000	0.583474000
1	-3.559710000	2.481259000	1.437607000
1	4.505743000	1.054731000	-0.385238000
8	3.557874000	1.245466000	-0.361918000
1	3.480608000	2.190238000	-0.557877000
12	2.005180000	-0.029646000	-0.162131000